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应变松弛下铁电薄膜尺寸效应的相场模拟

Phase Field Modeling the Size Effect of Ferroelectric Thin
Films by Considering the Relaxation of the Strain

张春祖

指导教师姓名: 周志东 副教授

专 业 名 称: 力 学

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**Phase Field Modeling the Size Effect of Ferroelectric Thin
Films by Considering the Relaxation of the Strain**

A Thesis Submitted to
the Graduates School in Partial Fulfillment of the Requirements
for the Degree of Master of Engineering

By

Chun-Zu ZHANG

Supervised by

Zhi-Dong ZHOU

Department of Civil Engineering

School of Architecture and Civil Engineering

Xiamen University

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摘要

钙钛矿型铁电薄膜材料具有铁电性、热电性、光电性、光折变性等多种性能，被越来越多的应用于微电子领域，成为制作非易失存储器、场效应管和热电传感器等的主要材料。但铁电薄膜厚度一般在微米以下，此时薄膜的尺寸效应很强，研究铁电薄膜材料的尺寸效应具有实际的理论和应用意义。

本文基于金茨堡-朗道-德文希尔（GLD）唯象理论框架，利用等效应变模型考虑薄膜内应变松弛，同时还结合薄膜表面晶格变化引起的极化改变和表面电荷引起的退极化效应等机电耦合边界条件，应用相场法建立了金茨堡-朗道-德文希尔时间发展方程。通过线性假设分析求解了顺电相向铁电相转变初始阶段居里温度随薄膜厚度的变化，并通过有限差分法数值求解了铁电薄膜的相变温度，铁电性，相结构类型与稳定性与薄膜厚度，机电耦合边界条件等的依赖关系。结果显示，铁电薄膜在尺寸较小时，机电耦合边界条件作用明显，而尺寸较大时，薄膜性能接近于块体材料，机电耦合边界条件影响较小，即尺寸效应不明显。机电耦合边界条件是影响铁电薄膜性能尺寸效应的主要因素，而各个因素之间的相互竞争决定了薄膜的最终性能。通过分析发现，当薄膜厚度较小时，薄膜表面极化改变和电极引起的退极化效应主导薄膜铁电性的尺寸效应，而薄膜厚度较大时，薄膜内应变松弛效应是铁电薄膜铁电性趋于块体材料铁电性的主要因素。由于薄膜内存在应变松弛效应，在温度不是很高时，首次得到了较厚单畴铁电薄膜在高拉应变区会出现稳定的 c 相。

对薄膜尺寸效应的分析具有实际指导意义。在实际的制备过程中，选择合适的基底可以得到性能最佳的铁电薄膜，也可通过选择生长合适的薄膜厚度，从而达到性能最佳和体积较小高集成的效果。同时，本文还提出了薄膜的铁电性，相结构和稳定性是多种边界相互竞争下的表现，进而完善了铁电薄膜相图。

关键词：铁电薄膜；尺寸效应；应变松弛；相场法

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Abstract

Ferroelectric thin films have been considerable importance in nonvolatile memory, field effect transistor, thermoelectric transducer and so on due to the ferroelectricity, thermoelectricity, photoelectricity and photorefractive properties. Generally, size effect is strong as the thickness of the films is always on nanoscale. So the investigations in this filed are significant.

Basing on the Ginzburg-Landau-Devonshire (GLD) theory, the time evolution equations of GLD are obtained by considering the “effective” strain model which considers relaxation of the internal strain, together with the surface eigenstrain relaxation and depolarization field. The size effect of the transition temperature, ferroelectricity and phase stability of the ferroelectric thin films are simulated, via the analytic solutions of linear hypothesis and numerical solutions by finite difference method. The results show that the effect of the boundary conditions is obvious when the thickness of the ferroelectric thin films is small. As the thickness growing, the properties of the films are closed to the bulk and the effect of the boundary conditions is weaken, which means the size effect is weak. The boundary conditions are the principal factors of the properties of the ferroelectric thin films, and the competition between the factors decides the properties. At the small scale, the effect of the surface lattice relaxation and the electrode induced depolarization is primary. When the thickness is large enough, the effect of the relaxation of the internal strain becomes primary. It is noteworthy, at low temperature, the stability c-phase is obtained at the high tension strain because of the relaxation of the internal strain.

In summary, the analysis of the size effect of ferroelectric thin films has practical significance. We can choose the appropriate thickness and the suitable substrates to design and grow the desired ferroelectric films. Here, the works also complete the phase diagrams of ferroelectric thin film.

Key words: ferroelectric thin films, size effect, relaxation of strain, phase field method

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目录

| | |
|---------------------------------------------|-----|
| 摘要..... | I |
| Abstract..... | III |
| 第一章 绪论 | 1 |
| 1.1 铁电材料的基本特性 | 1 |
| 1.2 铁电薄膜的应用 | 2 |
| 1.3 研究基本理论 | 3 |
| 1.3.1 金茨堡—朗道—德文希尔理论和相场法..... | 3 |
| 1.3.2 软模理论和 Ising 模型..... | 4 |
| 1.3.3 第一性原理..... | 5 |
| 1.4 铁电薄膜的发展现状 | 5 |
| 1.5 论文的研究内容及创新点 | 8 |
| 第二章 理论分析与模型建立 | 9 |
| 2.1 三维模型 | 9 |
| 2.2 一维模型 | 12 |
| 第三章 居里温度的线性化分析 | 14 |
| 3.1 线性化假设 | 14 |
| 3.2 变量分离求解 | 14 |
| 3.3 数值结果与分析 | 16 |
| 3.3.1 薄膜厚度对相变温度的影响..... | 17 |
| 3.3.2 表面极化改变与电荷屏蔽效应对相变温度的影响（机电耦合边界条件） | 18 |
| 3.3.3 内应变效应对相变温度的影响（机械边界条件） | 21 |
| 3.4 本章小结 | 22 |
| 第四章 铁电性能尺寸效应的非线性分析 | 24 |
| 4.1 有限差分方程 | 24 |
| 4.2 数值结果与分析 | 26 |

| | |
|---------------------------------|-----------|
| 4.2.1 温度对铁电性能的影响..... | 26 |
| 4.2.2 薄膜厚度对铁电性能的影响..... | 28 |
| 4.2.3 错配应变对铁电性能的影响..... | 29 |
| 4.2.4 表面晶格松弛和退极化效应对铁电性能的影响..... | 31 |
| 4.3 本章小结 | 32 |
| 第五章 单畴铁电薄膜的相结构与稳定性 | 34 |
| 5.1 有限差分方程 | 34 |
| 5.2 数值结果与分析 | 37 |
| 5.2.1 错配应变—温度相图分析..... | 38 |
| 5.2.2 错配应变—厚度相图分析..... | 41 |
| 5.3 本章小结 | 45 |
| 结论与展望..... | 46 |
| 参考文献..... | 48 |
| 攻读硕士期间发表的论文 | 53 |
| 致谢..... | 54 |

Table of Contents

| | |
|------------------------------------------------------------------------------------------------------------------|------------|
| Abstract in Chinese | I |
| Abstract..... | III |
| Chapter 1 Introduction | 1 |
| 1.1 Fundamental Characteristics of Ferroelectric Material | 1 |
| 1.2 Application of Ferroelectric Thin Films | 2 |
| 1.3 Basic Theories of Research..... | 3 |
| 1.3.1 Theory of Ginzburg-Landau-Devonshire and Phase Field Method | 3 |
| 1.3.2 Theory of Soft Mode and Ising Model | 4 |
| 1.3.3 First Principle | 5 |
| 1.4 Status of Ferroelectric Thin Films | 5 |
| 1.5 Content and Innovation of the Research | 8 |
| Chapter 2 Theories Discussing and Models Building..... | 9 |
| 2.1 3 Dimensional Model | 9 |
| 2.2 1 Dimensional Model | 12 |
| Chapter 3 Linear analysis of Curie Temperature..... | 14 |
| 3.1 Linear Hypothesis | 14 |
| 3.2 Solution of Separation of Variables..... | 14 |
| 3.3 Numerical Results and Discussion..... | 16 |
| 3.3.1 Effect of Film Thickness on Phase Transition Temperature | 17 |
| 3.3.2 Effect of Surface Eigenstrain Relaxation and Depolarization Field on Phase Transition Temperature | 18 |
| 3.3.3 Effect of Internal Strain on Phase Transition Temperature | 21 |
| 3.4 Brief Summary | 22 |
| Chapter 4 Nonlinear Analysis of Size Effect of Ferroelectricities | 24 |
| 4.1 Equations of Finite Difference | 24 |
| 4.2 Numerical Results and Discussion..... | 26 |

| | | |
|-------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------|-----------|
| 4.2.1 | Effect of Temperature on the Ferroelectricities..... | 26 |
| 4.2.2 | Effect of Film Thickness on the Ferroelectricities | 28 |
| 4.2.3 | Effect of Misfit Strain on the Ferroelectricities | 29 |
| 4.2.4 | Effect of Surface Eigenstrain Relaxation and Depolarization Field on the Ferroelectricities..... | 31 |
| 4.3 | Brief Summary | 33 |
| Chapter 5 Phase Stability of Single Domain Epitaxial Ferroelectric films | | 34 |
| 5.1 | Equations of Finite Difference | 34 |
| 5.2 | Numerical Results and Discussion..... | 37 |
| 5.2.1 | Discussion of the Phase Diagrams of Misfit Strain-Temperature | 38 |
| 5.2.2 | Discussion of the Phase Diagrams of Misfit Strain-Thickness | 41 |
| 5.3 | Brief Summary | 45 |
| Conclutions and Prospect..... | | 46 |
| References | | 48 |
| Publications during the Course of the Work..... | | 53 |
| Acknowledgements..... | | 54 |

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